## Response to Reviewer 3 Comments (RC3) for ESSD-2024-26

We thank you for your comments on our manuscript and suggestions for improving our work. We have addressed all the comments. Our response (AC) to each reviewer comment (RC) are shown in bold text below.

Best regards,

Anatol Helfenstein, on behalf of all authors

## General comments

Helfenstein et al. present a soil modelling and mapping platform for the Netherlands (BIS-4D). It "delivers maps of soil texture (clay, silt and sand content), bulk density, pH, total nitrogen, oxalate-extractable phosphorus, cation exchange capacity and their uncertainties at 25 m resolution between 0 - 2 m depth in 3D space. Additionally, it provides maps of soil organic matter and its uncertainty in 3D space and time between 1953 - 2023 at the same resolution and depth range." (see Abstract).

For the prediction of the maps, random forest (RF) and quantile regression forest (QRF) were used. Depending on the target variable 20-50 covariates were selected from a total of 366 environmental covariates. Predecessor versions of the method and the pH map were presented and published before (Helfenstein et al., 2022).

Together with the manuscript, the authors provide (i) the BIS-4D maps, (ii) the code to produce the maps, (iii) the soil point data that was used as target variables in the calibration of the models, and (iv) the majority of the covariates that were used in the modeling in raster format at 25 m resolution (excluding the non-openly available data). The code is very well documented, in a clear format, clearly structured in a series of scripts and well-arranged presented at the archive. The data sets are very well and clearly documented as well. All assets were easy to access via the given identifier and ready to apply.

The method is clearly presented and it is well conceivable that the BIS-4D platform will be used in the future to update the maps, produce maps of other soil properties or further develop the mapping method.

The manuscript is well written, good to follow and the line of thoughts and arguments is comprehensible. There are a few sentences and transitions between paragraphs that made me stumble. I addressed those and provided suggestions in the specific comments.

In general, I think it is an impressive and extensive piece of work that deserves publication.

## <u>AC:</u> Thank you very much for your positive feedback and taking the time to go through the manuscript and assets (data sets and code) in detail.

## Specific comments

(1) Median predictions

My understanding is that you used random forest (RF) for the mean predictions and quantile regression forest (QRF) with the 0.50 quantile for the median predictions. However, I did not find it explicitly stated. Maybe, I overread it. If not, please, include it.

<u>AC:</u> Please see L227, where we wrote: "For model calibration and prediction, we used RF to predict the mean and quantile regression forest (QRF) due to its ability to predict the entire conditional distribution (Meinshausen, 2006)". The entire probability distribution also includes the median, as you noted.

#### (2) Prediction in different depths

I understood it such that you used all soil observations for RF model tuning (L214-218) and calibrating the final RF and QRF models (L227-230). Then you used the calibrated RF and QRF to predict the target variables for the chosen depths (L240ff). If this is correct, can you please rephrase L214-218. As it is now, I find it confusing. Here, one suggestion:

"For model calibration, we used RF to predict the mean and quantile regression forest (QRF) to predict the entire conditional distribution (Meinshausen, 2006). The final models were fitted using all soil observations in the calibration set (Table 2), the selected covariates (Table 5) and the final set of hyper-parameters (Table 6).

## <u>AC:</u> We see that based on the quoted text the reviewer is referring to L227-230. We will change the text as you suggested, i.e. change "The final QRF" to the "the final models", since as you correctly state it was both RF and QRF models.

#### (3) Bias of predictions

L326-332: You measured the bias with the mean error (ME). Based on that you conclude "mean predictions were less biased than median predictions for all soil properties except SOM (Table 7)." and elaborate on the systematic differences between the bias of mean and median predictions.

My interpretation of the results is different. I would say, (a) the biases measured with ME are rather small for both, and as a result, (b) also the differences in bias measured with ME are rather small. More importantly, there are (c) systematic differences in the accuracy plots from the supplement, which are the other way round. The low and high values of the mean predictions are systematically biased such that the low values of the observed variable are overestimated, the high values underestimated. The median predictions are systematically less biased in this regard. This holds for all target variables, even though to different degree.

Thus, while the mean predictions are slightly less biased than the median predictions when averaging over all values, they are clearly more biased than the median predictions for the low and high values. Maybe, it is an effect of RF emphasizing the intermediate values? For my taste, the benefit with respect to the low and high values outweighs the slight gain with respect to the mean bias. RMSE and MEC are also quite on the same level for both variants. In summary, I would rather recommend to use the median predictions.

Can you please include the raised aspects (a-c) in your discussion and adapt your recommendation in case you find it appropriate?

## <u>AC:</u> Thank you for this comment and in-depth analysis. We very much agree with the reviewer and think this is an important improvement of the analysis of the results. We will change the text of this paragraph as follows (L326-332):

"The differences in accuracy between mean and median prediction maps varied slightly between soil properties. The low and high values of the mean predictions were systematically biased such that the low values of the observed soil property were overestimated and the high values underestimated, to varying degrees for different target soil properties (Fig. S10, S21, S32, S43, S54, S65, S76, S87 & S98). Thus, while the mean predictions were slightly less biased than the median predictions when averaging over all values, except for SOM (Table 7), they were more biased than the median predictions for the low and high values. For soil properties where calibration data were positively skewed (Fig. 3), i.e. all soil properties except sand, BD and pH, the bias of mean predictions was negative, whereas the bias of median predictions was positive (Table 7). In contrast to the findings based on 10-fold cross-validation, design-based inference of N<sub>tot</sub> revealed that median predictions were less biased (between -609 and 120 mg/kg; SI) than mean predictions (between -511 and -1408 mg/kg; SI). Higher accuracy of median predicted N<sub>tot</sub> was also reflected in lower RMSE (Table S7) and higher MEC values (Table 8). In summary, although it depends on the use, overall we recommend to use median predictions since low and high values were less biased and ME, RMSE and MEC values for both mean and median predictions were similar."

(4) Merging of data and comments in the scripts

Obviously, the quality of the data is vital for your work. This includes the quality of the chemical analysis as well as the preprocessing of the data. A major aspect is the correct merging of data from different sources. This I cannot evaluate, but it seems that for yourself there are still some questions marks.... At least there are some in the R-scripts in the code-repository associated with the submitted manuscript and data (https://git.wur.nl/helfe001/bis-4d). If you clarified the issues, great! If you did not, but the questionable variable is excluded for other reasons anyways, also great! In those cases, please simply update the comments in your scripts. If there are still open questions with variables that you use, especially the target variables, I think it would be of major importance to clarify those. Having written that, I am optimistic that it is merely a matter of updating the scripts.

At this point I like to take the opportunity to acknowledge strongly the effort you spend to put all the data together, document it clearly and provide it together with the well written and documented scripts in an easily accessible way. I know how cumbersome work it is. Big thumbs up!

In particular, I stumbled in the script 11\_soil\_PFB\_BPK\_LSK\_prep.R upon:

- •L73+338: If there are still open questions with PFB\_CHE it might be better to exclude it?
- •L259ff: If the difference between values of duplicate samples are large, it might be better simply to exclude both.
- •L1058: The old variable name sounds rather different ("CEC\_eff = SOM\_KAT"). Is this correctly assigned?

<u>AC:</u> Thank you for your suggestions and positive feedback on the work we did. I agree it's a good idea to remove some of the comments in the scripts which might confuse readers or people who want to use the scripts. We will do so for the final version. Regarding the specific comments the reviewer came across, the issues with PFB\_CHE have been solved so we will remove this comment. Large differences in values of duplicate samples were indeed excluded. Effective cation exchange capacity (CEC\_eff) was correctly assigned, as in Dutch it stands for "kationuitwisselcapaciteit ongebufferd". Assigning soil properties and renaming them to English was done in close collaboration with the database maintainers and soil surveyors (L121).

(5) Depth variables

Could you please elaborate why you included "the upper and lower boundary and midpoint of each sampled horizon" (L197)? What is the benefit over using just one depth variable? And if

there is one, why not just use two depth variables? If you have two of them, the third is already defined, similarly, like it is for the particle size fractions.

## AC: This was investigated in Ma et al. (2021), please see

10.1016/j.geoderma.2020.114794, Sect. 2.4.2. The effect of including boundaries in addition to midpoint was that it led to more "stepped" predictions. Furthermore, when including both upper and lower boundaries, the model can potentially also account for depth thicknesses, although it we can only speculate if RF does this. However, this was not the focus of this study, so we would prefer not to elaborate more on this and other users can easily apply our methodology with only the midpoint, for example.

## (6) Extreme values

Can you please discuss the extreme low values of pH, BD and CEC, and the extreme high values of Ntot (Table 2) being used in the calibration data?

And concerning the BD values, how was such precision (0.1) measured in the field?

<u>AC:</u> Our general approach to eliminating potential outliers was that there needs to be proof that the extreme value was an outlier and can be eliminated. Extreme values that for which no such proof was found were kept in the dataset to prevent data manipulation and support objectivity of the analysis. This was one criterium investigated in the exploratory analysis scripts of BIS-4D (scripts starting with "15\_soil\_BIS\_expl\_analysis..."). Therefore, such low values might seem unlikely but they are not impossible and if no evidence was found to remove them, they were kept. For example, pH [KCI] values of 0.9 have been measured in extremely acid heathland environments with sandy soils in the Netherlands. Bulk densities (BD) of 0.1 may be possible if it is 100% peat. Extremely high total N and CEC values are possible on agricultural parcels with very high fertilizer inputs. Regarding BD, these were also measured in the laboratory by weighing the dried soil divided by the known volume core. Including the known volume core will be added to the description of Table 1, as suggested by reviewer 2 (David Rossiter).

(7) Variable importance plots

I found it interesting that for all of your target variables, except clay, there were only one or two variables outstanding in the variable importance plots. Could you please add a few lines about those best predictors and the respective soil property like you did for Pox in L508ff. (silt + sand: meststoffen\_bgdm1993\_25m, fgr\_25m; BD: bodem50\_2021\_peatcode\_25m; SOM: peat\_xydt\_25m; pH: fgr\_25m; Ntot: bodem50\_2021\_peatcode\_25m).

<u>AC:</u> We appreciate the interest of the reviewer, but the aim of this manuscript was developing a general modelling framework and achieving high prediction accuracy, rather than model inference. Therefore, we prefer not to extend the length of the article but explaining these covariates in more detail. A general description of these covariates is included in Table 5 and more details can be found in the dataset of covariates and code repository provided alongside the manuscript. For model inference, there are more refined ways from the domain of explainable machine learning, such as biplots, partial dependence plots or Shapley values. Solely based on permutation or impurity metrics as provided in this manuscript, a more detailed analysis of the covariates seems highly speculative.

(8) Smaller number of covariates

Did you compare the performances from the current set-up with a set-up with a more rigorously limited number of covariates? For example, by decreasing the cut-off value for the correlated variables to |0.8| or |0.7|. If yes, could you please add a few lines why you chose the current set-up. If no, just take it as a comment for future work / updates of BIS-4D. It might be also interesting for comparison with other methods, like deep learning methods (see your statement in L525: "... deep learning has only outperformed ensemble decision tree models when using a small number of covariates...".).

# <u>AC:</u> The cutoff value of 0.8 for the Pearson correlation coefficient was based on the value used in Poggio et al., 2021 (DOI: 10.5194/soil-7-217-2021). We did not compare it with other cutoff values but would be happy if other studies would like to compare this. However, we think that the recursive feature elimination (RFE) step after de-correlation might play a larger role in determining the final covariates chosen for model calibration and prediction.

L10+11: Please rephrase such, that it is clear that, depending on the target variable, 20-50 environmental covariates were selected for each model from the 366 available ones.

<u>AC:</u> We have spent a lot of time writing and re-writing this sentence to try to make it concise and clear. We decided to keep it as it is because all 366 covariates were considered in the modelling process, even if only 20-50 are selected in the final model. One of the strength of BIS-4D is the amount of data prepared for improving the performance, so we want to emphasize this in the abstract.

Section 1 Introduction: Generally, well written, providing reasonable storyline and context.

L33-36: The last two sentences of the first paragraph are a little bit long and convoluted. Also, if "achieving a comprehensive understanding of soil spatial variability" would require a "high sampling density", it would kind of thwart your DSM approach. Please, rewrite the two sentences. For example, something like:

"Consequently, achieving a comprehensive understanding of soil spatial variability demands a high spatial resolution. The inherent difficulty, time consumption, and expense associated with collecting soil samples is thereby posing a major challenge for the task of mapping soils in 3D space and time (3D+T)."

<u>AC:</u> We will change the text to the following to make it more concise and less convoluted:

# "Fully grasping soil spatial variability requires dense sampling, but this is hindered by the difficulty, time, and expense of collecting soil samples. These challenges underscore the complexity of quantifying soil variation, highlighting the formidable task of mapping soils in 3D space and time (3D+T)."

L37: If you follow my suggestion above, I further suggest to start the new paragraph with "However, with the raising awareness ..."

## <u>AC:</u> We prefer to not start the new paragraph with "however" as it is a new idea and also not in direct contrast to the previous paragraph.

L37: What you mean with stakeholders like "value chains"?

<u>AC:</u> We agree this is not quite correct, as it reads not as if value chains were a stakeholder. We will change the sentence as follows: "With the rising awareness of soil health among diverse stakeholders and within value chains (Lehmann et al.,

## 2020), soil scientists are increasingly dedicated to deliver high-resolution, accurate soil maps."

Section 2.1 Soil point data: Nice overview and comprehensible placement of your work.

L150ff: Please provide a brief english description of the BPK and PFB data sets (samples from boreholes versus pits) as it is done in the README.md at https://git.wur.nl/helfe001/bis-4d.

# <u>AC:</u> According to database maintainers and soil surveyors, there are not only soil samples from boreholes in BPK and not only soil samples from soil pits in the PFB. These names and abbreviations were chosen decades ago and are a little confusing and do not help the reader if an English description would be provided.

L275-278: Well written. I like that you explicitly did the qualitative evaluation as well, and that you acknowledged its limitations.

L339-354: Well elaborated.

L350-352: And lack of predictors / variables that describe urban effects / disturbances.

# <u>AC:</u> Although we agree with the reviewer that there was a lack of covariates as specific proxies of urban effects and disturbances, these would be of little use if there are not observation locations from these areas because then they are also not captured in model training. Therefore, we maintain that the main reason is limited soil samples in urban areas, as currently written.

L377-378: Good to point out that "the mineral soil component should be used with caution in peatlands..."

L377-391: The provided information is clearly written and of high practical value.

L389-391: Another option would be to exclude the coordinates completely. If your idea is correct, the artifacts should vanish. Did you ever try that? It might be interesting to try it for future updates of BIS-4D. If the artifacts would vanish and if the performance of the prediction would not decrease substantially, excluding the coordinates would be the most straightforward solution.

# <u>AC:</u> We are open if future modelling studies would like to investigate this further, although this was largely already done by Møller et al., 2020 (<u>https://doi.org/10.5194/soil-6-269-2020</u>). They were beneficial for performance, otherwise they would not have been chosen as final covariates during RFE (L208-213).

L396: The point "4) the benefits of machine learning combined with large amounts of data" is already spelled out in the other points. Or is there some other benefit from the machine learning? If so, please name it explicitly. If not, point 4) can be deleted.

## <u>AC:</u> We disagree with the reviewer that point 4) is already included in the other points (1-6) in the sentence in L394-398. "The benefits of machine learning combined with large amounts of data" is not related to any of the following:

- the ability to provide information of soil properties as opposed to soil types
- the high spatial resolution (25m)
- accuracy and uncertainty assessment based on best practices
- the flexibility to predict in 3D and 3D+T

## • model code and data are openly available, making BIS-4D fully reproducible and easy to update

## Therefore, we will keep the sentence as it is currently written (L394-398).

L399-416: Well put into context.

L452-454: These two sentences feel a little convoluted for me. Please rephrase. Maybe also give examples of the innovative covariates that were used. Also, "Finally" is followed by "Lastly" in the following paragraph. Maybe replace "Finally" with, for example, "In addition".

<u>AC:</u> We will replace "Finally" with "In addition" as suggested by the reviewer in L452. The examples of innovative covariates that were developed for modelling soil organic matter in 3D+T are provided in the citation given in this sentence (Helfenstein et al., 2024c; DOI: 10.1038/s43247-024-01293-y).

L463-465: The sentence doubles with the sentence before. Please, rephrase / shorten it.

<u>AC:</u> We agree with the reviewer that his sentence is too much repetition with the previous and we have decided the rephrase this paragraph as follows (L462-465):

"Uncertainty in DSM products such as BIS-4D can be linked to three overarching sources: 1) the quantity and quality of soil point data, 2) the quantity and quality of covariates, and 3) the model structure (Heuvelink, 2014, 2018). In the following, we discuss the limitations of BIS-4D maps with regard to these three sources of uncertainty and suggest improvements."

L488-491: Good point.

Section 3.3.2 Covariates: Well reasoned.

Section 3.4. Assessment scale: Very important, well-founded and well written section of high practical value!

L576: I think this section is of high practical value and it makes sense to include it. However, as it is now, I recommend to sharpen it. For my understanding this is not a user manual. It is a mix of guidelines how to decide whether BIS-4D is helpful for the user's intended purpose and recommendations how to use BIS-4D. Please, change the section title according to your intention and rephrase the text of the section accordingly, as well as L18 in the abstract. This affects also the following comment. Both comments can be handled together.

<u>AC:</u> Thank you for the suggestion. As this was also remarked by reviewer 2 (David Rossiter), we will change the title of Sect. 3.5 to "Best practices for proper use". We think with this change in the title of the section, the text fits well, so we will not change it. However, we will also adjust the text in the abstract (L18) to "We describe best practices to help users decide whether BIS-4D is suitable for their intended purpose, ..."

L577-581: The first paragraph of the "BIS-4D user manual" should be moved somewhere else or substantially rephrased. My guess is, that the idea was to give some general recommendations which of the maps are considered reliable enough for which purpose. As it is now, you give only one such recommendation for Pox (and not several, as the beginning of the following paragraph is suggesting).

<u>AC:</u> We agree this could be improved. We think that by changing the section title much confusion is resolved. Furthermore, we will include the first sentence of the second paragraph (L582-583) in the first paragraph and remove the phrase "Beyond these general recommendations". This will result in the following:

"For  $P_{ox}$ , we only recommend the produced maps for a qualitative overview of  $P_{ox}$  spatial distribution in the Netherlands. We have summarized the following simple chronological steps for users to help decide whether BIS-4D maps may be suitable for their intended purpose: ...".

L580: Please, include "qualitative". For example: "we only recommend it for a qualitative overview of its spatial distribution in the Netherlands."

## <u>AC:</u> We will add the word "qualitative" as suggested by the reviewer, see comment directly above.

## Technical comments and suggestions

Use the percentage sign consistently with or without leading space. I personally prefer with leading space ("X %").

## <u>AC:</u> According to ESSD submission guidelines (https://www.earth-system-sciencedata.net/submission.html#math), we agree that there should be a space and will adjust this throughout the manuscript

L18-20: I would prefer four sentences, instead of one long one. Simply replace the "," and the last ", and" with ".".

## <u>AC:</u> We agree this sentence is too long and will change it to three short sentences as follows (L18-21):

"A step-by-step manual helps users decide whether BIS-4D is suitable for their intended purpose. An overview of all maps and their uncertainties can be found in the supplementary information (SI). Openly available code and input data enhance reproducibility and future updates. BIS-4D prediction maps can be readily downloaded at https://doi.org/10.4121/ 20 0c934ac6-2e95-4422-8360-d3a802766c71 (Helfenstein et al., 2024a)."

L20: Delete "easily" or replace with "readily".

## AC: We will adjust this as suggested (see above).

L30: "making it less mobile and unable to form"

## AC: We will adjust it as suggested.

L37-44 (paragraph 2): I would delete the last sentence and change the end of the first sentence to: "(Lehmann et al., 2020), there is an increasing demand for accurate high-resolution soil maps to facilitate land use decisions and management practices at multiple scales."

## <u>AC:</u> We have already improved this paragraph (see comments above) and will therefore not adjust it further.

L56: I think "crop" can be deleted.

## AC: We agree and will remove the word "crop".

L73-93: For me, these two paragraphs feel a bit like jumping back and forth. Maybe, simply change the order of the two paragraphs. Then, it is first the story of the Netherlands and its soil mapping, which transitions to the story of DSM.

<u>AC:</u> We have spent considerable effort structuring the order of these paragraphs. At one point, I presented a version to my co-authors with the structure you propose (paragraph 6 followed by paragraph 5) and compared it to the current structure (paragraph 5 followed by 6), but we decided to use the current structure. This structure is more intuitive and "expected", as we first provide a general overview of soil maps and DSM worldwide (paragraph 5), followed by soil maps and DSM in the Netherlands (paragraph 6).

L95: "Even though DSM has established itself and is routinely implemented across the world, various challenges remain."

## <u>AC:</u> We think it is better to use the transition word in the second clause of the sentence rather than starting a new paragraph with a transitioning phrase ("even though").

L101: "related"

## AC: We will change "relating" to "related".

L101+102: "... 5 and 9), in particular that the uncertainty of soil maps is often not quantified..."

## AC: We will change it as you suggest. Thank you for the suggestion.

L104: "However, assessing map accuracy, ..."

## AC: We think moreover fits better here than however.

L110: "consistent" can be deleted

## AC: We will delete that word.

L122: "assessed" (I guess)

## AC: We will change it to past tense (assessed) as suggested.

Fig2: Why "per 3 km2"? Please add space in front of "km".

## AC: We will add the space.

L185: "preferable"

## AC: We will change "preferential" to "preferable".

L204: You mean "design matrix"?

## <u>AC:</u> We are certain that "regression matrix" is the correct term in this context, as widely used and defined in statistical modelling (and digital soil mapping).

L281: " the here presented version"

## AC: We will change "this version" to "the here presented version".

L298: "..., while..."

## AC: We will add the comma in front of "while".

L548: Can be shortened, for example: "Many potential users of BIS-4D may require information specifically for one land use or soil type."

## AC: We will shorten it as suggested.

L551-554: Convoluted sentence, please rephrase in shorter sentences. As it is now, probably an "in" is missing after "interested"?

## <u>AC:</u> Thank you for catching the error. Indeed, the word "in" is missing.

L557: Maybe replace "above a certain threshold" with "high enough".

## AC: We will replace it as suggested.

L601: "for the intended purpose"

## AC: We will change it as suggested.

## Supplements

Variable importance-plots: Consider scaling the variable importances such, that they sum up to 100 % (or 1 if you prefer that). It simplifies reading / comparing the results.

<u>AC:</u> We disagree that changing the scale of the x-axis in the variable importance plots simplifies the reading and helps with comparing the results. The variable importance plots simply show the relative importance of each covariate. However, the absolute values on the x-axis by themselves are insignificant and should also not be compared between models (e.g. variable importance value of covariate XY in the clay model with variable importance value of covariate XY in the pH model).

Figure S55: Empty page on S37.

## AC: We will adjust the formatting. Thank you for the suggestion.

Figure S98: "CEC" in the labels of the x-axis.

<u>AC:</u> The labels on the x-axis in the supplementary figure S98 are already "CEC" so we do not understand this comment of the reviewer. The hat (" $^{"}$ ) on "CEC" implies that they are predictions (in contrast to the observations on the y-axis) and is undisputed statistical notation and also used in all other predicted vs. observed plots in the supplements.

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## Comments to the code repository (https://git.wur.nl/helfe001/bis-4d)

(1) Very good that you provide EDA plots, in particular that you produced maps to identify spatial clustering / bias. In addition, I recommend to include in future work / updates of BIS-4D:

(a) time series of the target variables, to see whether there are obvious shifts or trends, and

(b) a check whether the value distributions of the target variables differ substantially between the data sources (BPK, LSK, PFB), for example with histograms or boxplots.

<u>AC:</u> Thank you for your comments and suggestions. If the reviewer is suggesting time series of target soil properties at point locations, that is not possible because there is not monitoring data with sufficient quality at point support in the Netherlands (L490-491). However, BIS-4D does include space-time mapping in 3D+T (SOM maps in data assets and Helfenstein et al., 2024c, which is now published (DOI: 10.1038/s43247-024-01293-y)). This is discussed and referenced throughout the entire manuscript. This is also included in the code. We already compared distributions of calibration (BPK and PFB) and validation (LSK and CCNL) data using histograms and boxplots. See scripts starting with "15\_soil\_BIS\_expl\_analysis\_target..." and scripts 35 for pH and SOM. For example, see L183 in exploratory analysis script

"15\_soil\_BIS\_expl\_analysis\_target\_sand.Rmd" for a histogram of PFB laboratory measurements of sand content. Furthermore, PFB and LSK or CCNL data are also directly compared using histograms in script "35\_model\_data\_expl\_analysis.Rmd" (code chunks starting at L205 and L502, respectively).

## (2) Broken links:

In README.md / master level - "Model workflow (R scripts), 1. Soil data preparation":

- •15\_soil\_BIS\_expl\_analysis\_LSK\_CCNL.Rmd
- •15\_soil\_BIS\_expl\_analysis\_target\_SOC\_SOM.Rmd
- •16\_soil\_BIS\_remove\_Ohorizon\_outliers.R
- •22\_cov\_cat\_recl\_gdal\_par.R
- 30\_regression\_matrix.R
- •40\_train\_RF\_LLO\_KFCV\_hyperparameter\_tuning.R
- •41\_train\_QRF\_LLO\_KFCV\_optimal\_model.R
- 50\_model\_evaluation\_all\_depths\_PFB-OOB\_PFB-CV\_LSK.R
- •51\_model\_evaluation\_depth\_layers\_PFB-OOB\_PFB-CV\_LSK\_LSK-SRS.R
- •60\_predict\_QRF\_soil\_maps.R
- •61\_map\_soil\_properties.R
- •target\_prediction\_depth\_GSM.R
- out/data/covariates/DEM\_derivatives
- out/maps/other/SoilGrids\_v2.0/SoilGrids\_phh2o\_model\_evaluation\_LSK\_SRS\_d.csv
- out/maps/target/pH\_KCl/GeoTIFFs
- out/maps/target/pH\_KCl/pdf

In "https://git.wur.nl/helfe001/bis-4d/-/blob/master/25\_cov\_expl\_analysis\_clorpt.Rmd":

• https://git.wur.nl/helfe001/bis-4d/-/blob/master/img/landuse\_ede\_wageningen\_hgn.jpg

# <u>AC:</u> Thank you for the reminder. These links will be fixed. As written in the first sentences of the README.md, "This README is currently a duplicate of the BIS-3D README, which comes along the public release of the Helfenstein et al., 2022 manuscript. As such, this README is not yet complete, as some scripts, files and directories are missing a description." This will be done for the final publication.

(3) In section "Summary of supporting scripts, files and directories": Maybe rename the second sub bullet "covariates" listed under bullet "data" to "other"

## <u>AC:</u> Ah indeed we noticed that both bullets under "data" are called "covariates". We will change one of these names.

(4) In the script https://git.wur.nl/helfe001/bis-4d/-/blob/master/20\_cov\_prep\_gdal.R it says:

# make noise raster, which we will later use for (ad-hoc) feature elimination: # all covariates less important (permutation/impurity) than noise covariate in RF # can be removed in final model calibration

Is this used? If not, please remove it or add a comment in the script. If it is used, please add a comment in the manuscript.

<u>AC:</u> This was used in the earlier development stages of BIS-4D but now the "noise" covariate is no longer used for ad-hoc feature elimination, so we will remove this comment to avoid confusion.